FILE 'HCAPLUS' ENTERED AT 11:51:40 ON 04 JUN 2004

=> d his ful

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E PRIESTLEY E SCOTT/AU
L1
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                E DECICCO CARL P/AU
            123 SEA ABB=ON ("DECICCO C P"/AU OR "DECICCO CARL"/AU OR "DECICCO
                CARL P"/AU OR "DECICCO CARL PETER"/AU)
              4 SEA ABB=ON L1 AND L2
L3
                SELECT RN L3 1-4
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                42918-86-5/BI OR 4333-56-6/BI OR 460-
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L6
               STR
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FILE 'HCAPLUS' ENTERED AT 12:22:40 ON 04 JUN 2004
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0 SEA SSS SAM L6

1 SEA SSS FUL L6

0 SEA SSS SAM L9

STR L6

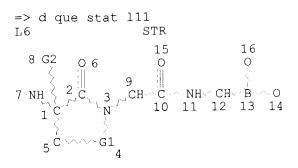
L7

 $\Gamma8$ 

L9L10

L11

FILE 'CAOLD' ENTERED AT 12:49:26 ON 04 JUN 2004
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REP G1=(1-3) CH2 VAR G2=H/C NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

L8 1 SEA FILE=REGISTRY SSS FUL L6
L11 2 SEA FILE=HCAPLUS ABB=ON L8

### => d ibib abs hitstr l11 1-2

L11 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:23525 HCAPLUS

DOCUMENT NUMBER:

138:90078

TITLE:

Preparation of lactam acylaminoalkaneboronates as

inhibitors of hepatitis C virus NS3 protease.

INVENTOR(S):

Priestley, E. Scott; Decicco, Carl P.

PATENT ASSIGNEE(S):

SOURCE:

U.S. Pat. Appl. Publ., 45 pp., Cont.-in-part of U.S.

Ser. No. 626,286, abandoned.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE US 2003008828 A1 20030109 US 2001-10184 20011206 PRIORITY APPLN. INFO.: US 1999-145631P P 19990726 US 2000-626286 B2 20000725

OTHER SOURCE(S): MARPAT 138:90078

AB Title compds. I [X = B(OH)2, BY1Y2, COCONHR1a; Y1, Y2 = OH, F, amino, alkoxy; BY1Y2 = atoms to form a cyclic boron ester, amide, or amide-ester containing 2-20 C atoms and optionally 1-3 N, O, or S atoms; R1, R1a = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl; R2 = H; R1R2C = cycloalkyl; R3 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, Ph, naphthyl, heteroaryl; R4 = H, (substituted) alkyl, Ph, PhCH2, PhCH2CH2; R5 = H, QR5a; Q = chain of 0-3 amino acids; R5a = SOR6, SO2R6, COR6, CO2R8, etc.; R6 = (substituted) alkyl, Ph, naphthyl, PhCH2, heteroaryl; R8 = alkyl, PhCH2, cycloalkylmethyl; Z = (CH2)1-3] were prepared as inhibitors of hepatitis C virus NS3 protease. Thus, (1R)-1-[[(2S)-3-cyclohexyl-2-[3isopropyl-3-[[(2S)-3-methyl-2-[(2-pyrazinylcarbonyl)amino]butanoyl]amino]-2-oxo-1-pyrrolidinyl]propanoyl]amino]-3-butenylboronic acid (+)-pinanediol ester was prepared by solution phase chemical A number of I inhibited hepatitis C

virus NS3 protease with Ki <60  $\mu M$ .

#### 323196-93-6P IT

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(preparation of lactam acylaminoalkaneboronates as inhibitors of hepatitis C virus NS3 protease)

RN 323196-93-6 HCAPLUS

CN Boronic acid, [(1R)-1-[[(2S)-3-cyclohexyl-2-[3-(1-methylethyl)-3-[[(3-methylethyl)-3-[](3-methylethyl)]] methylphenyl)sulfonyl]amino]-2-oxo-1-pyrrolidinyl]-1oxopropyl]amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L11 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: DOCUMENT NUMBER:

2001:78359 HCAPLUS

DOCOME

134:147855

CODEN: PIXXD2

TITLE:

Preparation of lactam acylaminoalkaneboronates as

inhibitors of hepatitis C virus NS3 protease.

INVENTOR(S):

Priestley, E. Scott; Decicco, Carl P. Du Pont Pharmaceuticals Company, USA

PATENT ASSIGNEE(S): SOURCE:

PCT Int. Appl., 130 pp.

DOCUMENT TYPE: Pa

LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KI				KI	KIND DATE				APPLICATION NO.				DATE					
Ţ	wo	0 2001007407			A1 20010201				WO 2000-US20189					20000726				
		W:	ΑU,	BR,	CA,	CN,	CZ,	EE,	HU,	ΙL,	IN,	JP,	KR,	LT,	LV,	MX,	NO,	NZ,
			PL,	RO,	SG,	SI,	SK,	TR,	UA,	VN,	ZA,	AM,	AZ,	BY,	KG,	KZ,	MD,	RU,
			ТJ,														·	
		RW:	AT,	BE,	CH,	CY,	DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙĖ,	ΙT,	LU,	MC,	NL,
			PT,	SE														
EP 1206449 A								EP 2000-950642 20000726										
		R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
			ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL							
PRIORITY APPLN. INFO.:				J				JS 1999-145631P			Р	19990726						
								•	1	WO 20	7-00C	JS20	189	W	2000	0726		
OTHER SOURCE(S): GI					MARPAT 134:147855													

AΒ Title compds. [I; X = B(OH)2, BYY1, COCONHRla; Y1, Y2 = OH, F, amino, alkoxy; BY1Y2 = atoms to form a cyclic boron ester, amide, or amide-ester containing 2-20 C atoms and optionally 1-3 N, O, or S atoms; R1, R1a = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl; R2 = H; R1R2C = cycloalkyl; R3 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, Ph, naphthyl, heteroaryl; R4 = H, (substituted) alkyl, Ph, PhCH2, PhCH2CH2; R5 = H, QR5a; Q = chain of 0-3 amino acids; R5a = SOR6, SO2R7, COR6, CO2R8; R6 = (substituted) alkyl, Ph, naphthyl, PhCH2, heteroaryl; R7 = H, alkyl; R8 = alkyl, PhCH2, cycloalkylmethyl; Q = (CH2)1-3], were prepared Thus, (1R) -1 - [[(2S) -3 - cyclohexyl -2 - [3 - isopropyl -3 - [[(2S) -3 - methyl -2 - [(2 - isopropyl -3 - [(2S) -3 - methyl -2 - [(2 - isopropyl -3 - [(2S) -3 - methyl -2 - [(2S) -3 pyrazinylcarbonyl)amino]butanoyl]amino]-2-oxo-1pyrrolidinyl]propanoyl]amino]-3-butenylboronic acid (+)-pinanediol ester was prepared by solution phase chemical A number of I inhibited hepatitis C virus

NS3 protease with Ki<60  $\mu$ M.

#### 323196-93-6P ΙT

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of lactam acylaminoalkaneboronates as inhibitors of hepatitis C virus NS3 protease)

323196-93-6 HCAPLUS RN

CN Boronic acid, [(1R)-1-[(2S)-3-cyclohexyl-2-[3-(1-methylethyl)-3-[(3-methyl)-3-[(3-methyl)-3-[(3-methyl)-3-[(3-methyl)-3-[(3-mmethylphenyl)sulfonyl]amino]-2-oxo-1-pyrrolidinyl]-1oxopropyl]amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT Lukton 10/010,184

04/06/2004

=> d ibib abs hitstr 15 1-4

ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2003:23525 HCAPLUS

DOCUMENT NUMBER:

138:90078

TITLE:

Preparation of lactam acylaminoalkaneboronates as

inhibitors of hepatitis C virus NS3 protease.

INVENTOR(S):

Priestley, E. Scott; Decicco, Carl

PATENT ASSIGNEE(S):

USA

SOURCE:

U.S. Pat. Appl. Publ., 45 pp., Cont.-in-part of U.S.

Ser. No. 626,286, abandoned.

CODEN: USXXCO

DOCUMENT TYPE:

Patent English

LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO. DATE
US 2003008828	A1	20030109	US 2001-10184 20011206
PRIORITY APPLN. INFO.	:		US 1999-145631P P 19990726
INTORITI III III.			us 2000-626286 B2 20000725

OTHER SOURCE(S):

MARPAT 138:90078

GT

Title compds. I [X = B(OH)2, BY1Y2, COCONHR1a; Y1, Y2 = OH, F, amino, ΔR alkoxy;  $B\bar{Y}1Y2$  = atoms to form a cyclic boron ester, amide, or amide-ester containing 2-20 C atoms and optionally 1-3 N, O, or S atoms; R1, R1a = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl; R2 = H; R1R2C = cycloalkyl; R3 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, Ph, naphthyl, heteroaryl; R4 = H, (substituted) alkyl, Ph, PhCH2, PhCH2CH2; R5 = H, QR5a; Q = chain of 0-3 amino acids; R5a = SOR6, SO2R6, COR6, CO2R8, etc.; R6 = (substituted) alkyl, Ph, naphthyl, PhCH2, heteroaryl; R8 = alkyl, PhCH2, cycloalkylmethyl; Z = (CH2)1-3] were prepared as inhibitors of hepatitis C virus NS3 protease. Thus, (1R)-1-[[(2S)-3-cyclohexyl-2-[3-4cm-representation of the company of the cycloal state of the cyc isopropyl-3-[[(2S)-3-methyl-2-[(2-pyrazinylcarbonyl)amino]butanoyl]amino]-2-oxo-1-pyrrolidinyl]propanoyl]amino]-3-butenylboronic acid (+)-pinanediol ester was prepared by solution phase chemical A number of I inhibited hepatitis C

virus NS3 protease with Ki <60  $\mu M$ .

149885-80-3 ΙT

RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)

(inhibitors; preparation of lactam acylaminoalkaneboronates as inhibitors of hepatitis C virus NS3 protease)

149885-80-3 HCAPLUS RN

Proteinase, polyprotein-processing, NS3 (9CI) (CA INDEX NAME) CN

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

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323196-84-5P 323196-85-6P 323196-86-7P
ΙT
    323196-87-8P 323196-88-9P 323196-89-0P
    323196-90-3P 323196-91-4P 323196-92-5P
    323196-93-6P 323196-94-7P 323196-95-8P
    323196-96-9P 323196-97-0P 323196-98-1P
    323196-99-2P 323197-00-8P 323197-01-9P
    323197-02-0P 323197-03-1P 323197-04-2P
    323197-05-3P 323197-06-4P 323197-07-5P
    323197-08-6P 323197-09-7P
    RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
    (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
    (Uses)
       (preparation of lactam acylaminoalkaneboronates as inhibitors of hepatitis C
       virus NS3 protease)
    323196-84-5 HCAPLUS
RN
    CN
    [(3aS, 4S, 6S, 7aR) -hexahydro-3a, 5, 5-trimethyl-4, 6-methano-1, 3, 2-
    benzodioxaborol-2-yl]-3-butenyl]amino]-2-oxoethyl]-3-(1-methylethyl)-2-oxo-
    3-pyrrolidinyl]amino]carbonyl]-2-methylpropyl]- (9CI) (CA INDEX NAME)
```

Absolute stereochemistry.

$$H_2C$$
 $H_3C$ 
 $H_4C$ 
 $H_5C$ 
 $H_6C$ 
 $H_7C$ 
 $H_7C$ 

RN 323196-85-6 HCAPLUS
CN Pyrazinecarboxamide, N-[(1S)-1-[[[1-[(1S)-1-(cyclohexylmethyl)-2-[[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]-3-butenyl]amino]-2-oxoethyl]-3-(1-methylethyl)-2-oxo-3-piperidinyl]amino]carbonyl]-2-methylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323196-86-7 HCAPLUS
CN 1H-Azepine-1-acetamide, N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]hexahydro-3-[(methylsulfonyl)amino]-2-oxo-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323196-87-8 HCAPLUS

CN 1-Pyrrolidineacetamide, 3-amino-α-(cyclohexylmethyl)-N-[(1R)-1[(3as,4s,6s,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-2-oxo-, monohydrochloride,
(αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 323196-88-9 HCAPLUS

CN 1-Pyrrolidineacetamide, 3-[([1,1'-biphenyl]-4-ylsulfonyl)amino]-α-(cyclohexylmethyl)-N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-2-oxo-, (αS)-(9CI) (CA INDEX NAME)

RN 323196-89-0 HCAPLUS

CN 1-Pyrrolidineacetamide,  $\alpha$ -(cyclohexylmethyl)-N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-2-oxo-3-[[(4-propylphenyl)sulfonyl]amino]-,  $(\alpha S)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323196-90-3 HCAPLUS

CN 1-Pyrrolidineacetamide,  $\alpha$ -(cyclohexylmethyl)-N-[(1R)-1-[(3aS, 4S, 6S, 7aR)-hexahydro-3a, 5, 5-trimethyl-4, 6-methano-1, 3, 2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-3-[(1-naphthalenylsulfonyl)amino]-2-oxo-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

RN 323196-91-4 HCAPLUS

CN 1-Pyrrolidineacetamide,  $\alpha$ -(cyclohexylmethyl)-N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-2-oxo-3-[[(phenylamino)carbonyl]amino]-,  $(\alpha S)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323196-92-5 HCAPLUS

CN 1-Pyrrolidineacetamide,  $\alpha$ -(cyclohexylmethyl)-N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-3-[[(3-methylphenyl)sulfonyl]amino]-2-oxo-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323196-93-6 HCAPLUS

CN Boronic acid, [(1R)-1-[[(2S)-3-cyclohexyl-2-[3-(1-methylethyl)-3-[[(3-methylphenyl)sulfonyl]amino]-2-oxo-1-pyrrolidinyl]-1-oxopropyl]amino]propyl]- (9CI) (CA INDEX NAME)

RN 323196-94-7 HCAPLUS

CN Carbamic acid, [1-[(1S)-2-[[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]amino]-2-oxo-1-phenylethyl]-3-(1-methylethyl)-2-oxo-3-pyrrolidinyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323196-95-8 HCAPLUS

CN 1-Pyrrolidineacetamide, 3-amino-N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-2-oxo-α-phenyl-, monohydrochloride, (αS)- (9CI) (CA INDEX NAME)

HC1

RN 323196-96-9 HCAPLUS

CN 1-Pyrrolidineacetamide, N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-metháno-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-3-[(methylsulfonyl)amino]-2-oxo-α-phenyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN . 323196-97-0 HCAPLUS

Absolute stereochemistry.

Pr-n

RN 323196-98-1 HCAPLUS

CN Carbamic acid, [1-[(1S)-1-[[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-[(3aS,4S,6S,7aR)-hexahydro-3a,5-[(3aS,4S,5]-hexahydro-3a,5-[(3aS,4S,5]-hexahydro-3a,5-[(3a

trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]amino]carbonyl]-3methylbutyl]-3-(1-methylethyl)-2-oxo-3-pyrrolidinyl]-, phenylmethyl ester
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323196-99-2 HCAPLUS

CN 1-Pyrrolidineacetamide, 3-amino-N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-α-(2-methylpropyl)-2-oxo-, monohydrochloride, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 323197-00-8 HCAPLUS

CN 1-Pyrrolidineacetamide, N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)- $\alpha$ -(2-methylpropyl)-3-[(methylsulfonyl)amino]-2-oxo-, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

RN 323197-01-9 HCAPLUS

CN 1-Pyrrolidineacetamide, N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-α-(2-methylpropyl)-2-oxo-3-[[(4-propylphenyl)sulfonyl]amino]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-02-0 HCAPLUS

CN Pyrazinecarboxamide, N-[(1S)-1-[[[1-[(1S)-1-(cyclohexylmethyl)-2-[[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]-3-butenyl]amino]-2-oxoethyl]-3-ethyl-2-oxo-3-pyrrolidinyl]amino]carbonyl]-2-methylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-03-1 HCAPLUS

CN Carbamic acid, [1-[(1S)-1-(cyclohexylmethyl)-2-[[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]amino]-2-oxoethyl]-3-(1-methylethyl)-2-oxo-3-piperidinyl]-,

phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-04-2 HCAPLUS

CN Carbamic acid, [1-[(1S)-2-[[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]amino]-2-oxo-1-phenylethyl]-3-(1-methylethyl)-2-oxo-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-05-3 HCAPLUS

1-Piperidineacetamide, 3-amino-N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-2-oxo-α-phenyl-, monohydrochloride, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 323197-06-4 HCAPLUS

CN Carbamic acid, [1-[(1S)-2-[[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]amino]-2-oxo-1-phenylethyl]-3-(1-methylethyl)-2-oxo-3-piperidinyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-07-5 HCAPLUS

CN 1-Piperidineacetamide, 3-(benzoylamino)-N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-2-oxo- $\alpha$ -phenyl-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-08-6 HCAPLUS

CN 1-Piperidineacetamide, N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-3-[(methylsulfonyl)amino]-2-oxo- $\alpha$ -phenyl-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

RN 323197-09-7 HCAPLUS

CN 1-Piperidineacetamide, N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-3-[[(3-methylphenyl)sulfonyl]amino]-2-oxo- $\alpha$ -phenyl-, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

85-46-1, 1-Naphthylsulfonyl chloride 98-88-4, Benzoyl ΙT chloride 103-71-9, Phenyl isocyanate, reactions 106-95-6 , Allyl bromide, reactions 108-98-5, Thiophenol, reactions 124-63-0, Methanesulfonyl chloride 359-07-9 460-37-7, 3,3,3-Trifluoropropyl iodide 931-59-9, Phenylsulfenyl chloride 1149-26-4 1623-93-4, 4-Biphenylsulfonyl chloride 1730-25-2, Allylmagnesium bromide **1899-93-0 3182-79-4 4333-56-6,** Cyclopropyl bromide 6009-07-0 13734-41-3 15028-39-4, L-Phenylglycine methyl ester hydrochloride 17193-39-4 18680-27-8 38329-34-9, L-Phenylglycine hydrochloride 42918-86-5 76347-13-2 84110-32-7 90084-27-8 119479-32-2 130653-09-7 146949-07-7 323197-58-6 323197-73-5 RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of lactam acylaminoalkaneboronates as inhibitors of hepatitis C virus NS3 protease) RN 85-46-1 HCAPLUS 1-Naphthalenesulfonyl chloride (7CI, 8CI, 9CI) (CA INDEX NAME) CN

RN 98-88-4 HCAPLUS CN Benzoyl chloride (8CI, 9CI) (CA INDEX NAME)

RN 103-71-9 HCAPLUS

CN Benzene, isocyanato- (9CI) (CA INDEX NAME)

RN 106-95-6 HCAPLUS

CN 1-Propene, 3-bromo- (9CI) (CA INDEX NAME)

Br-CH2 CH-CH2

RN 108-98-5 HCAPLUS

CN Benzenethiol (8CI, 9CI) (CA INDEX NAME)



RN 124-63-0 HCAPLUS

CN Methanesulfonyl chloride (6CI, 8CI, 9CI) (CA INDEX NAME)

RN 359-07-9 HCAPLUS

CN Ethane, 2-bromo-1,1-difluoro- (7CI, 8CI, 9CI) (CA INDEX NAME)

RN 460-37-7 HCAPLUS

CN Propane, 1,1,1-trifluoro-3-iodo- (7CI, 8CI, 9CI) (CA INDEX NAME)

F3C-CH2-CH2I

RN 931-59-9 HCAPLUS

CN Benzenesulfenyl chloride (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

 ${\rm Ph^-\,S^-\,Cl}$ 

RN 1149-26-4 HCAPLUS

CN L-Valine, N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 1623-93-4 HCAPLUS

CN [1,1'-Biphenyl]-4-sulfonyl chloride (9CI) (CA INDEX NAME)

RN 1730-25-2 HCAPLUS

CN Magnesium, bromo-2-propenyl- (9CI) (CA INDEX NAME)

H<sub>2</sub>C— CH— CH<sub>2</sub>— Mg— Br

RN 1899-93-0 HCAPLUS

CN Benzenesulfonyl chloride, 3-methyl- (9CI) (CA INDEX NAME)

RN 3182-79-4 HCAPLUS

CN Glycine, N-2-propenyl-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{O} \\ \parallel \\ \text{EtO} \cdot \text{C---} \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{CH-----} \text{CH}_2 \end{array}$$

RN 4333-56-6 HCAPLUS

CN Cyclopropane, bromo- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

A Br

RN 6009-07-0 HCAPLUS

CN Disulfide, chloro phenyl (8CI, 9CI) (CA INDEX NAME)

Phs -S-Cl

RN 13734-41-3 HCAPLUS

CN L-Valine, N-[(1,1-dimethylethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 15028-39-4 HCAPLUS

CN Benzeneacetic acid,  $\alpha$ -amino-, methyl ester, hydrochloride,  $(\alpha S)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

● HCl

RN 17193-39-4 HCAPLUS

CN Cyclohexanepropanoic acid,  $\alpha$ -amino-, methyl ester, hydrochloride,  $(\alpha S)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

## ● HCl

RN 18680-27-8 HCAPLUS CN Bicyclo[3.1.1]heptane-2,3-diol, 2,6,6-trimethyl-, (1S,2S,3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 38329-34-9 HCAPLUS

CN Benzeneacetic acid,  $\alpha$ -amino-, hydrochloride,  $(\alpha S)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

# ● HCl

RN 42918-86-5 HCAPLUS

CN Butanoic acid, 2-[[(phenylmethoxy)carbonyl]amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 76347-13-2 HCAPLUS

CN 1,3,2-Dioxaborolane, 4,4,5,5-tetramethyl-2-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 84110-32-7 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole, 2-ethenylhexahydro-3a,5,5-trimethyl-, (3aS,4S,6S,7aR)~ (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 90084-27-8 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole, 2-[(1S)-1-chloro-2-(phenylmethoxy)ethyl]hexahydro-3a,5,5-trimethyl-, (3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 119479-32-2 HCAPLUS

CN 4-Pentenoic acid, 2-[[(1,1-dimethylethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)

RN 130653-09-7 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole, 2-(1-chloroethenyl)hexahydro-3a,5,5-trimethyl-, (3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

RN 146949-07-7 HCAPLUS

CN Benzenesulfonyl chloride, 4-propyl- (9CI) (CA INDEX NAME)

RN 323197-58-6 HCAPLUS

CN L-Valine, N-(pyrazinylcarbonyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-73-5 HCAPLUS

CN: 4,6-Methano-1,3,2-benzodioxaborole-2-methanamine, hexahydro-3a,5,5-trimethyl- $\alpha$ -2-propenyl-, ( $\alpha$ R,3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

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ΙΤ
     66080-23-7P 66866-64-6P 70557-99-2P
     83622-42-8P 94242-86-1P 95656-94-3P
     126689-01-8P 131357-48-7P 131433-93-7P
     172096-96-7P 319009-74-0P 319009-76-2P
     319009-78-4P 319009-80-8P 319009-82-0P
     319009-90-0P 319009-92-2P 319009-94-4P
     319009-96-6P 319009-98-8P 319010-99-6P
     319011-02-4P 319011-08-0P 319011-10-4P
     319011-16-0P 319011-18-2P 319011-22-8P
     319011-25-1P 319011-27-3P 319011-29-5P
     323197-10-0P 323197-11-1P 323197-12-2P
     323197-13-3P 323197-14-4P 323197-15-5P
     323197-16-6P 323197-17-7P 323197-18-8P
     323197-19-9P 323197-20-2P 323197-21-3P
     323197-22-4P 323197-23-5P 323197-24-6P
     323197-25-7P 323197-26-8P 323197-27-9P
     323197-28-0P 323197-29-1P 323197-30-4P
     323197-31-5P 323197-32-6P 323197-33-7P
     323197-34-8P 323197-35-9P 323197-36-0P
     323197-37-1P 323197-38-2P 323197-39-3P
     323197-40-6P 323197-41-7P 323197-42-8P
     323197-43-9P 323197-44-0P 323197-45-1P
    323197-46-2P 323197-47-3P 323197-48-4P
     323197-74-6P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of lactam acylaminoalkaneboronates as inhibitors of hepatitis C
        virus NS3 protease)
RN
    66080-23-7 HCAPLUS
CN
    1,3,2-Dioxaborolane, 4,4,5,5-tetramethyl-2-[(phenylthio)methyl]- (9CI)
     (CA INDEX NAME)
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RN 66866-64-6 HCAPLUS
CN 3-Oxazolidinecarboxylic acid, 4-(1-methylethyl)-5-oxo-, phenylmethyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 70557-99-2 HCAPLUS CN 1,3,2-Dioxaborolane, 2-(iodomethyl)-4,4,5,5-tetramethyl- (9CI) (CA INDEX

NAME)

RN 83622-42-8 HCAPLUS
CN 1,3,2-Dioxaborolane, 2-(chloromethyl)-4,4,5,5-tetramethyl- (9CI) (CA INDEX NAME)

RN 94242-86-1 HCAPLUS
CN 1,3,2-Dioxaborolane, 2-(1-chloroethyl)-4,4,5,5-tetramethyl- (9CI) (CA INDEX NAME)

RN 95656-94-3 HCAPLUS
CN 3-Oxazolidinecarboxylic acid, 4-ethyl-5-oxo-, phenylmethyl ester, (4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 126689-01-8 HCAPLUS
CN 1,3,2-Dioxaborolane, 2-cyclopropyl-4,4,5,5-tetramethyl- (9CI) (CA INDEX NAME)

RN 131357-48-7 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole, 2-[(1S)-1-chloro-3-butenyl]hexahydro-3a,5,5-trimethyl-, (3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 131433-93-7 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole, hexahydro-3a,5,5-trimethyl-2-(2-propenyl)-, (3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 172096-96-7 HCAPLUS

Absolute stereochemistry. Rotation (+).

RN 319009-74-0 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole-2-methanamine, hexahydro-3a,5,5-

trimethyl- $\alpha$ -[1-(phenylmethoxy)ethyl]-, hydrochloride, ( $\alpha$ R, 3aS, 4S, 6S, 7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 319009-76-2 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole-2-methanamine, hexahydro-3a,5,5-trimethyl- $\alpha$ -[(phenylmethoxy)methyl]-, hydrochloride, ( $\alpha$ R,3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 319009-78-4 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole-2-methanamine, hexahydro-3a,5,5-trimethyl- $\alpha$ -[(phenylthio)methyl]-, hydrochloride, (3aS,4S,6S,7aR)-(9CI) (CA INDEX NAME)

HCl

RN 319009-80-8 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole-2-methanamine, hexahydro-3a,5,5-trimethyl- $\alpha$ -[(phenyldithio)methyl]-, (3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 319009-82-0 HCAPLUS

CN 1,3,2-Dioxaborolane-2-methanamine, 4,4,5,5-tetramethyl- $\alpha$ -(3,3,3-trifluoropropyl)- (9CI) (CA INDEX NAME)

RN 319009-90-0 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole-2-methanamine, hexahydro-3a,5,5-trimethyl- $\alpha$ -2-propenyl-, hydrochloride, ( $\alpha$ R,3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

● HCl

RN 319009-92-2 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole-2-methanamine,  $\alpha$ -ethylhexahydro-3a,5,5-trimethyl-, hydrochloride, ( $\alpha$ R,3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 319009-94-4 HCAPLUS

CN 1,3,2-Dioxaborolane-2-methanamine,  $\alpha$ -cyclopropyl-4,4,5,5-tetramethyl-(9CI) (CA INDEX NAME)

RN 319009-96-6 HCAPLUS

CN 1,3,2-Dioxaborolane-2-methanamine,  $\alpha$ -(2,2-difluoroethyl)-4,4,5,5-tetramethyl-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 319009-98-8 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole-2-methanamine,  $\alpha$ -ethenylhexahydro-3a,5,5-trimethyl-, hydrochloride, ( $\alpha$ R,3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 319010-99-6 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole, 2-[(1S)-1-chloropropyl]hexahydro-3a,5,5-trimethyl-, (3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 319011-02-4 HCAPLUS

CN 1,3,2-Dioxaborolane, 2-(chlorocyclopropylmethyl)-4,4,5,5-tetramethyl-(9CI) (CA INDEX NAME)

RN 319011-08-0 HCAPLUS

CN 1,3,2-Dioxaborolane, 2-[3,3-difluoro-1-(phenylthio)propyl]-4,4,5,5-tetramethyl- (9CI) (CA INDEX NAME)

RN 319011-10-4 HCAPLUS

CN 1,3,2-Dioxaborolane, 2-(3,3-difluoro-1-iodopropyl)-4,4,5,5-tetramethyl-(9CI) (CA INDEX NAME)

RN 319011-16-0 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole, hexahydro-3a,5,5-trimethyl-2-[1-(phenylmethoxy)ethyl]-, (3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 319011-18-2 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole, 2-[(1S)-1-chloro-2-(phenylmethoxy)propyl]hexahydro-3a,5,5-trimethyl-, (3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 319011-22-8 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole, 2-[1-chloro-2-(phenylthio)ethyl]hexahydro-3a,5,5-trimethyl-, (3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 319011-25-1 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole, 2-[1-chloro-2-(phenyldithio)ethyl]hexahydro-3a,5,5-trimethyl-, (3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 319011-27-3 HCAPLUS

CN 1,3,2-Dioxaborolane, 4,4,5,5-tetramethyl-2-[4,4,4-trifluoro-1-(phenylthio)butyl]- (9CI) (CA INDEX NAME)

RN 319011-29-5 HCAPLUS

CN 1,3,2-Dioxaborolane, 4,4,5,5-tetramethyl-2-(4,4,4-trifluoro-1-iodobutyl)(9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
Me & O & I \\
CH-CH_2-CH_2-CF_3
\end{array}$$
Me Me Me

RN 323197-10-0 HCAPLUS

CN 3-Oxazolidinecarboxylic acid, 4-(1-methylethyl)-5-oxo-4-(2-propenyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \circ \\ | \\ \mathsf{C}-\mathsf{O}-\mathsf{CH}_2-\mathsf{Ph} \\ | \\ \mathsf{Pr}-\mathsf{i} \\ \circ \\ \mathsf{CH}_2-\mathsf{CH}-\mathsf{CH}_2 \end{array}$$

RN 323197-11-1 HCAPLUS

CN 4-Pentenoic acid, 2-(1-methylethyl)-2-[[(phenylmethoxy)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 323197-12-2 HCAPLUS

CN Valine, 2-(2-oxoethyl)-N-[(phenylmethoxy)carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 323197-13-3 HCAPLUS

CN 1-Pyrrolidineacetic acid,  $\alpha$ -(cyclohexylmethyl)-3-(1-methylethyl)-2-oxo-3-[[(phenylmethoxy)carbonyl]amino]-, methyl ester, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-14-4 HCAPLUS

CN 1-Pyrrolidineacetic acid, 3-amino- $\alpha$ -(cyclohexylmethyl)-3-(1-methylethyl)-2-oxo-, methyl ester, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-15-5 HCAPLUS

CN 1-Pyrrolidineacetic acid,  $\alpha$ -(cyclohexylmethyl)-3-(1-methylethyl)-3-[(2S)-3-methyl-1-oxo-2-[(pyrazinylcarbonyl)amino]butyl]amino]-2-oxo-, methyl ester, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

RN 323197-16-6 HCAPLUS

CN 1-Pyrrolidineacetic acid,  $\alpha$ -(cyclohexylmethyl)-3-(1-methylethyl)-3-[(2S)-3-methyl-1-oxo-2-[(pyrazinylcarbonyl)amino]butyl]amino]-2-oxo-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-17-7 HCAPLUS

CN Norvaline, 5-hydroxy-2-(1-methylethyl)-N-[(phenylmethoxy)carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 323197-18-8 HCAPLUS

CN Norvaline, 2-(1-methylethyl)-5-oxo-N-[(phenylmethoxy)carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 323197-19-9 HCAPLUS

CN Cyclohexanepropanoic acid,  $\alpha$ -[[4-(methoxycarbonyl)-5-methyl-4-[[(phenylmethoxy)carbonyl]amino]hexyl]amino]-, methyl ester, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-20-2 HCAPLUS

CN 1-Piperidineacetic acid,  $\alpha$ -(cyclohexylmethyl)-3-(1-methylethyl)-2-oxo-3-[[(phenylmethoxy)carbonyl]amino]-, methyl ester, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-21-3 HCAPLUS

CN 1-Piperidineacetic acid, 3-amino- $\alpha$ -(cyclohexylmethyl)-3-(1-methylethyl)-2-oxo-, methyl ester, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

RN 323197-22-4 HCAPLUS

CN 1-Piperidineacetic acid,  $\alpha$ -(cyclohexylmethyl)-3-(1-methylethyl)-3-[(2S)-3-methyl-1-oxo-2-[(pyrazinylcarbonyl)amino]butyl]amino]-2-oxo-, methyl ester, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-23-5 HCAPLUS

CN 1-Piperidineacetic acid,  $\alpha$ -(cyclohexylmethyl)-3-(1-methylethyl)-3-[[(2S)-3-methyl-1-oxo-2-[(pyrazinylcarbonyl)amino]butyl]amino]-2-oxo-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-24-6 HCAPLUS

CN Glycine, 4,5-didehydro-N-[(1,1-dimethylethoxy)carbonyl]norvalyl-N-2-propenyl-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \circ & \circ \\ & \circ & \circ \\ \text{NH-C-OBu-t} \\ & | & | \\ \text{H}_2\text{C--CH-CH}_2 - \text{CH-CH}_2 - \text{CH--CH}_2 \\ & | & | \\ \text{EtO-C-CH}_2 \\ & | & | \\ \text{O} \end{array}$$

RN 323197-25-7 HCAPLUS

CN 1H-Azepine-1-acetic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2,3,4,7-tetrahydro-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)

RN 323197-26-8 HCAPLUS

CN 1H-Azepine-1-acetic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2,3,4,7-tetrahydro-2-oxo- (9CI) (CA INDEX NAME)

RN 323197-27-9 HCAPLUS

CN Carbamic acid, [1-[2-[[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]amino]-2-oxoethyl]hexahydro-2-oxo-1H-azepin-3-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-28-0 HCAPLUS

CN 1H-Azepine-1-acetamide, 3-amino-N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]hexahydro-2-

oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-29-1 HCAPLUS

CN 1-Pyrrolidineacetic acid,  $\alpha$ -(cyclohexylmethyl)-3-(1-methylethyl)-2-oxo-3-[[(phenylmethoxy)carbonyl]amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-30-4 HCAPLUS

CN Carbamic acid, [1-[(1S)-1-(cyclohexylmethyl)-2-[[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]amino]-2-oxoethyl]-3-(1-methylethyl)-2-oxo-3-pyrrolidinyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 323197-31-5 HCAPLUS

CN 1-Pyrrolidineacetic acid, 3-(1-methylethyl)-2-oxo- $\alpha$ -phenyl-3-[[(phenylmethoxy)carbonyl]amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-32-6 HCAPLUS

CN 1-Pyrrolidineacetic acid, 3-(1-methylethyl)- $\alpha$ -(2-methylpropyl)-2-oxo-3-[[(phenylmethoxy)carbonyl]amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-33-7 HCAPLUS

CN 3-Oxazolidinecarboxylic acid, 4-ethyl-5-oxo-4-(2-propenyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & \\ C-O & CH_2-Ph \\ & Et \\ O & CH_2-CH=-CH_2 \end{array}$$

RN 323197-34-8 HCAPLUS

CN 4-Pentenoic acid, 2-ethyl-2-[[(phenylmethoxy)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 323197-35-9 HCAPLUS

CN Butanoic acid, 2-ethyl-4-oxo-2-[[(phenylmethoxy)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 323197-36-0 HCAPLUS

CN 1-Pyrrolidineacetic acid,  $\alpha$ -(cyclohexylmethyl)-3-ethyl-2-oxo-3- [[(phenylmethoxy)carbonyl]amino]-, methyl ester, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

RN 323197-37-1 HCAPLUS

CN 1-Pyrrolidineacetic acid, 3-amino- $\alpha$ -(cyclohexylmethyl)-3-ethyl-2-oxo-, methyl ester, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-38-2 HCAPLUS

CN 1-Pyrrolidineacetic acid,  $\alpha$ -(cyclohexylmethyl)-3-ethyl-3-[[(2S)-3-methyl-1-oxo-2-[(pyrazinylcarbonyl)amino]butyl]amino]-2-oxo-, methyl ester, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

RN 323197-39-3 HCAPLUS

CN 1-Pyrrolidineacetic acid,  $\alpha$ -(cyclohexylmethyl)-3-ethyl-3-[[(2S)-3-methyl-1-oxo-2-[(pyrazinylcarbonyl)amino]butyl]amino]-2-oxo-, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-40-6 HCAPLUS

CN 3-Oxazolidinecarboxylic acid, 4-(1-methylethyl)-5-oxo-4-(2-propenyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
O \\
C \\
C \\
O \\
O
\end{array}$$

$$\begin{array}{c}
O \\
CH_2 - CH = CH_2
\end{array}$$

RN 323197-41-7 HCAPLUS

CN 4-Pentenoic acid, 2-[[(1,1-dimethylethoxy)carbonyl]amino]-2-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 323197-42-8 HCAPLUS

CN 4-Pentenoic acid, 2-[[(1,1-dimethylethoxy)carbonyl]amino]-2-(1-methylethyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{O} \\ \parallel \\ \text{C-O-CH}_2\text{-Ph} \\ \mid \\ \text{i-Pr} \quad \text{C-CH}_2\text{-CH--CH}_2 \\ \mid \\ \text{NH-C OBu-t} \\ \mid \\ \text{O} \end{array}$$

RN 323197-43-9 HCAPLUS

CN Norvaline, N-[(1,1-dimethylethoxy)carbonyl]-5-hydroxy-2-(1-methylethyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 323197-44-0 HCAPLUS

CN Norvaline, N-[(1,1-dimethylethoxy)carbonyl]-2-(1-methylethyl)-5-oxo-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 323197-45-1 HCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[[4-[[(1,1-dimethylethoxy)carbonyl]amino]-5-methyl-4-[(phenylmethoxy)carbonyl]hexyl]amino]-, methyl ester, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

RN 323197-46-2 HCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[[4-carboxy-4-[[(1,1-dimethylethoxy)carbonyl]amino]-5-methylhexyl]amino]-, monomethyl ester,  $(\alpha S)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-47-3 HCAPLUS

CN l-Piperidineacetic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-methylethyl)-2-oxo- $\alpha$ -phenyl-, methyl ester, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-48-4 HCAPLUS

CN 1-Piperidineacetic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-methylethyl)-2-oxo- $\alpha$ -phenyl-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-74-6 HCAPLUS

CN 1-Pyrrolidineacetic acid, 3-(1-methylethyl)-2-oxo-α-phenyl-3[[(phenylmethoxy)carbonyl]amino]-, methyl ester, (αS)- (9CI) (CA
INDEX NAME)

## IT 483387-26-4 483387-27-5 483387-28-6 483387-29-7

RL: PRP (Properties)

(unclaimed protein sequence; preparation of lactam acylaminoalkaneboronates as inhibitors of hepatitis C virus NS3 protease.)

RN 483387-26-4 HCAPLUS

CN Peptide, (Asp-Glu-Xaa-Glu-Xaa-Cys) (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 483387-27-5 HCAPLUS

CN Peptide, (Asp-Xaa-Ile-Val-Pro-Cys) (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 483387-28-6 HCAPLUS

CN Peptide, (Asp-Glu-Val-Pro-Xaa) (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 483387-29-7 HCAPLUS

CN Peptide, (Asp-Glu-Asp-Glu-Glu-Xaa-Ala-Ser-Lys) (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

## IT 204765-53-7 438493-18-6 483340-48-3 483340-49-4

RL: PRP (Properties)

(unclaimed sequence; preparation of lactam acylaminoalkaneboronates as inhibitors of hepatitis C virus NS3 protease.)

RN 204765-53-7 HCAPLUS

CN L-Lysine, L-lysyl-L-lysylglycyl-L-seryl-L-valyl-L-valyl-L-isoleucyl-L-valylglycyl-L-arginyl-L-isoleucyl-L-valyl-L-leucyl-L-serylglycyl-L-lysyl-L-prolyl-L-alanyl-L-isoleucyl-L-isoleucyl-L-prolyl-L-lysyl- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

PAGE 1-C

NH<sub>2</sub>

PAGE 2-D

NH2

(CH<sub>2</sub>) 4

RN 438493-18-6 HCAPLUS

CN L-Histidine, L-methionyl-L-arginylglycyl-L-seryl-L-histidyl-L-histidyl-L-histidyl-L-histidyl-L-histidyl-L-methionylglycyl-L-alanyl-L-glutaminyl- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

PAGE 1-C

RN 483340-48-3 HCAPLUS

CN L-Histidine, L-methionylglycyl-L-alanyl-L-glutaminyl- (9CI) (CA INDEX NAME)

483340-49-4 HCAPLUS RN

L-Cysteine, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L- $\alpha$ -glutamyl-L-CN alanyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2002:767330 HCAPLUS

DOCUMENT NUMBER:

138:221813

TITLE:

Pl Phenethyl peptide boronic acid inhibitors of HCV

NS3 protease

AUTHOR(S):

Priestley, E. Scott; De Lucca, Indawati; Ghavimi, Bahman; Erickson-Viitanen, Susan;

Decicco, Carl P.

CORPORATE SOURCE:

Experimental Station, Bristol-Myers Squibb

Pharmaceutical Research Institute, Wilmington, DE,

19880-0500, USA

SOURCE:

Bioorganic & Medicinal Chemistry Letters (2002),

12(21), 3199-3202

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER:

Elsevier Science Ltd.

DOCUMENT TYPE:

Journal

English

LANGUAGE:

A series of peptide boronic acids containing extended, hydrophobic Pl residues was prepared to probe the shallow, hydrophobic S1 region of HCV NS3 protease. The p-trifluoromethylphenethyl P1 substituent was identified as

```
optimal with respect to inhibitor potency for NS3 and selectivity against
     elastase and chymotrypsin.
     9004-06-2, Elastase 9004-07-3, Chymotrypsin
ΤТ
     149885-80-3, Ns3 protease
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (preparation of P1 phenethyl peptide boronic acid inhibitors of HCV NS3
        protease)
     9004-06-2 HCAPLUS
RN
     Elastase (9CI) (CA INDEX NAME)
CN
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
     9004-07-3 HCAPLUS
RN
CN
     Chymotrypsin (9CI) (CA INDEX NAME)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
     149885-80-3 HCAPLUS
RN
     Proteinase, polyprotein-processing, NS3 (9CI) (CA INDEX NAME)
CN
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
     500763-17-7P 500763-19-9P 500763-21-3P
     500763-23-5P 500763-25-7P 500763-27-9P
     500763-29-1P 500763-31-5P 500763-33-7P
     500763-35-9P 500763-37-1P 500763-39-3P
     500763-42-8P 500763-44-0P 500763-46-2P
     500763-48-4P 500763-50-8P 500763-52-0P
     500763-53-1P 500763-55-3P 500763-57-5P
     500763-59-7P 500763-61-1P 500763-63-3P
     500763-65-5P 500763-67-7P 500763-69-9P
     500763-71-3P 500763-73-5P 500763-74-6P
     500763-75-7P 500763-76-8P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
     (Biological study); PREP (Preparation)
        (preparation of P1 phenethyl peptide boronic acid inhibitors of HCV NS3
        protease)
     500763-17-7 HCAPLUS
RN
     L-Prolinamide, L-\alpha-aspartyl-L-\alpha-glutamyl-L-valyl-L-valyl-N-
CN
     [(1R)-1-[(3aS, 4S, 6S, 7aR)-hexahydro-3a, 5, 5-trimethyl-4, 6-methano-1, 3, 2-
     benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)
```

Absolute stereochemistry.

RN 500763-19-9 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS,4S,6S,7aR)-3a-butylhexahydro-5,5-dimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 500763-21-3 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-5,5-dimethyl-3a-pentyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 500763-23-5 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS,4S,6S,7aR)-3a-hexylhexahydro-5,5-dimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

RN 500763-25-7 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-5,5-dimethyl-3a-(2-methylpropyl)-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 500763-27-9 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS, 4S, 6S, 7aR)-hexahydro-5, 5-dimethyl-3a-(3-methylbutyl)-4, 6-methano-1, 3, 2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

RN 500763-29-1 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS, 4S, 6S, 7aR)-hexahydro-5, 5-dimethyl-3a-(4-methylpentyl)-4, 6-methano-1, 3, 2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 500763-31-5 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aR,4S,6S,7aR)-hexahydro-5,5-dimethyl-3a-phenyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

RN 500763-33-7 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS, 4S, 6S, 7aR)-hexahydro-5, 5-dimethyl-3a-(phenylmethyl)-4, 6-methano-1, 3, 2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 500763-35-9 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-5,5-dimethyl-3a-(2-phenylethyl)-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

RN 500763-37-1 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS, 4S, 6S, 7aR)-hexahydro-5, 5-dimethyl-3a-(3-phenylpropyl)-4, 6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 500763-39-3 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS, 4S, 6S, 7aR)-hexahydro-5, 5-dimethyl-3a-(4-phenylbutyl)-4, 6-methano-1, 3, 2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

RN 500763-42-8 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-5,5-dimethyl-3a-[2-(2-methylphenyl)ethyl]-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 500763-44-0 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-5,5-dimethyl-3a-[2-(3-methylphenyl)ethyl]-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

RN 500763-46-2 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-5,5-dimethyl-3a-[2-(4-methylphenyl)ethyl]-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

| Me

RN 500763-48-4 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS,4S,6S,7aR)-3a-[2-(2,4-dimethylphenyl)ethyl]hexahydro-5,5-dimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 2-A

| Me

RN 500763-50-8 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS, 4S, 6S, 7aR)-3a-[2-(2,5-dimethylphenyl)ethyl]hexahydro-5,5-dimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

RN 500763-52-0 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS, 4S, 6S, 7aR)-3a-[2-(2-fluorophenyl)ethyl]hexahydro-5,5-dimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 500763-53-1 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS,4S,6S,7aR)-3a-[2-(3-fluorophenyl)ethyl]hexahydro-5,5-

dimethy1-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 500763-55-3 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS,4S,6S,7aR)-3a-[2-(4-fluorophenyl)ethyl]hexahydro-5,5-dimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

| F

RN 500763-57-5 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS,4S,6S,7aR)-3a-[2-(2,6-difluorophenyl)ethyl]hexahydro-5,5-dimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

RN 500763-59-7 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-5,5-dimethyl-3a-[2-[3-(trifluoromethyl)phenyl]ethyl]-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 500763-61-1 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS, 4S, 6S, 7aR)-hexahydro-5, 5-dimethyl-3a-[2-[4-

(trifluoromethyl)phenyl]ethyl]-4,6-methano-1,3,2-benzodioxaborol-2yl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 2-A CF3

RN 500763-63-3 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS,4S,6S,7aR)-3a-[2-(4-chlorophenyl)ethyl]hexahydro-5,5-dimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

Cl

RN 500763-65-5 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS,4S,6S,7aR)-3a-[2-(4-bromophenyl)ethyl]hexahydro-5,5-dimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

Br

RN 500763-67-7 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS,4S,6S,7aR)-3a-(2-[1,1'-biphenyl]-4-ylethyl)hexahydro-5,5-dimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

| Ph

RN 500763-69-9 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-5,5-dimethyl-3a-[2-[4-(1-methylethyl)phenyl]ethyl]-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

i-Pr

RN 500763-71-3 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS,4S,6S,7aR)-3a-[2-(4-cyclohexylphenyl)ethyl]hexahydro-5,5-dimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)



RN 500763-73-5 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS,4S,6S,7aR)-3a-[2-[4-(1,1-dimethylethyl)phenyl]ethyl]hexahydr o-5,5-dimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

t-Bu

RN 500763-74-6 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a-[2-(4-hydroxyphenyl)ethyl]-5,5-dimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

OH

RN 500763-75-7 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N- [(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a-[2-(4-methoxyphenyl)ethyl]-5,5-dimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CI) (CA INDEX NAME)

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| OMe

RN 500763-76-8 HCAPLUS

CN L-Prolinamide, L-α-aspartyl-L-α-glutamyl-L-valyl-L-valyl-N[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-5,5-dimethyl-3a-[2-(4-phenoxyphenyl)ethyl]-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]- (9CT)
(CA INDEX NAME)

PAGE 2-A

| OPh

ΙT 98-80-6, Phenylboronic acid 100-58-3, Phenylmagnesium bromide 100-80-1, 3 Methylstyrene 350-51-6, 3 Fluorostyrene **394-46-7**, 2 Fluorostyrene **402-24-4**, 3 Trifluoromethylstyrene 402-50-6, 4 Trifluoromethylstyrene **405-99-2**, 4 Fluorostyrene **611-15-4**, 2 Methylstyrene **622-97-9,** 4 Methylstyrene **637-69-4,** 4 Methoxystyrene 693-03-8, Butylmagnesium bromide 693-25-4, Pentylmagnesium bromide 925-90-6, Ethylmagnesium bromide 926-62-5, Isobutylmagnesium bromide 1073-67-2, 4 Chlorostyrene 1462-75-5 1589-82-8, Benzylmagnesium bromide 1746-23-2, 4 tert Butylstyrene 2039-82-9, 4 Bromostyrene 2039-89-6, 2 5 Dimethylstyrene 2055-40-5, 4 Isopropylstyrene 2146-67-0, Dichloromethyllithium 2234-20-0, 2 4 Dimethylstyrene 2350-89-2, 4 Phenylstyrene 2628-17-3, 4 Hydroxystyrene 3277-89-2, Phenethylmagnesium bromide 3761-92-0, Hexylmagnesium bromide 4548-78-1, Isopentylmagnesium bromide 4973-29-9, 4 Phenoxystyrene 5419-55-6, Triisopropyl borate 7429-94-9 , 4-Methylpentylmagnesium bromide 13020-34-3, 4 Cyclohexylstyrene 18680-27-8 27152-04-1 207226-37-7, 2 6 Difluorostyrene 274918-51-3 RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of P1 phenethyl peptide boronic acid inhibitors of HCV NS3 protease)

RN 98-80-6 HCAPLUS

CN Boronic acid, phenyl- (9CI) (CA INDEX NAME)

RN 100-58-3 HCAPLUS

CN Magnesium, bromophenyl- (8CI, 9CI) (CA INDEX NAME)

Ph-Mg Br

RN 100-80-1 HCAPLUS

CN Benzene, 1-ethenyl-3-methyl- (9CI) (CA INDEX NAME)

RN 350-51-6 HCAPLUS

CN Benzene, 1-ethenyl-3-fluoro- (9CI) (CA INDEX NAME)

RN 394-46-7 HCAPLUS

CN Benzene, 1-ethenyl-2-fluoro- (9CI) (CA INDEX NAME)

RN 402-24-4 HCAPLUS

CN Benzene, 1-ethenyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 402-50-6 HCAPLUS

CN Benzene, 1-ethenyl-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 405-99-2 HCAPLUS CN Benzene, 1-ethenyl-4-fluoro- (9CI) (CA INDEX NAME)

CH-CH<sub>2</sub>

RN 611-15-4 HCAPLUS CN Benzene, 1-ethenyl-2-methyl- (9CI) (CA INDEX NAME)

CH— CH<sub>2</sub>

RN 622-97-9 HCAPLUS CN Benzene, 1-ethenyl-4-methyl- (9CI) (CA INDEX NAME)

CH -CH<sub>2</sub>

RN 637-69-4 HCAPLUS CN Benzene, 1-ethenyl-4-methoxy- (9CI) (CA INDEX NAME)

CH=CH<sub>2</sub>

RN 693-03-8 HCAPLUS CN Magnesium, bromobutyl- (8CI, 9CI) (CA INDEX NAME)

n-Bu-Mg-Br

RN 693-25-4 HCAPLUS CN Magnesium, bromopentyl- (7CI, 8CI, 9CI) (CA INDEX NAME) Me-(CH<sub>2</sub>)<sub>4</sub>-Mg-Br

RN 925-90-6 HCAPLUS

CN Magnesium, bromoethyl- (8CI, 9CI) (CA INDEX NAME)

H3C-CH2-Mq-Br

RN 926-62-5 HCAPLUS

CN Magnesium, bromo(2-methylpropyl) - (9CI) (CA INDEX NAME)

i-Bu-Mg-Br

RN 1073-67-2 HCAPLUS

CN Benzene, 1-chloro-4-ethenyl- (9CI) (CA INDEX NAME)

CH = CH<sub>2</sub>

RN 1462-75-5 HCAPLUS

CN Magnesium, bromo(3-phenylpropyl) - (8CI, 9CI) (CA INDEX NAME)

Ph- (CH2)3-Mg-Br

RN 1589-82-8 HCAPLUS

CN Magnesium, bromo(phenylmethyl) - (9CI) (CA INDEX NAME)

Ph-CH2 Mg Br

RN 1746-23-2 HCAPLUS

CN Benzene, 1-(1,1-dimethylethyl)-4-ethenyl- (9CI) (CA INDEX NAME)

t-Bu CH=CH2

RN 2039-82-9 HCAPLUS

CN Benzene, 1-bromo-4-ethenyl- (9CI) (CA INDEX NAME)

RN 2039-89-6 HCAPLUS CN Benzene, 2-ethenyl-1,4-dimethyl- (9CI) (CA INDEX NAME)

RN 2055-40-5 HCAPLUS CN Benzene, 1-ethenyl-4-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 2146-67-0 HCAPLUS CN Lithium, (dichloromethyl)- (7CI, 8CI, 9CI) (CA INDEX NAME)

RN 2234-20-0 HCAPLUS CN Benzene, 1-ethenyl-2,4-dimethyl- (9CI) (CA INDEX NAME)

RN 2350-89-2 HCAPLUS CN 1,1'-Biphenyl, 4-ethenyl- (9CI) (CA INDEX NAME)

RN 2628-17-3 HCAPLUS CN Phenol, 4-ethenyl- (9CI) (CA INDEX NAME)

RN 3277-89-2 HCAPLUS CN Magnesium, bromo(2-phenylethyl)- (9CI) (CA INDEX NAME)

Ph-CH<sub>2</sub>-CH<sub>2</sub>-Mg-Br

RN 3761-92-0 HCAPLUS CN Magnesium, bromohexyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

Me ( $CH_2$ ) 5 - Mg - Br

RN 4548-78-1 HCAPLUS
CN Magnesium, bromo(3-methylbutyl)- (9CI) (CA INDEX NAME)

 $Me_2CH-CH_2-CH_2-Mg-Br$ 

RN 4973-29-9 HCAPLUS CN Benzene, 1-ethenyl-4-phenoxy- (9CI) (CA INDEX NAME)

RN 5419-55-6 HCAPLUS CN Boric acid (H3BO3), tris(1-methylethyl) ester (9CI) (CA INDEX NAME)

RN 7429-94-9 HCAPLUS

Magnesium, bromo(4-methylpentyl)- (9CI) (CA INDEX NAME)

Me<sub>2</sub>CH- (CH<sub>2</sub>)<sub>3</sub>-Mg-Br

RN 13020-34-3 HCAPLUS

CN Benzene, 1-cyclohexyl-4-ethenyl- (9CI) (CA INDEX NAME)

H2C-

RN 18680-27-8 HCAPLUS

CN Bicyclo[3.1.1]heptane-2,3-diol, 2,6,6-trimethyl-, (1S,2S,3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

27152-04-1 HCAPLUS RN

CN Magnesium, bromo(4-phenylbutyl) - (8CI, 9CI) (CA INDEX NAME)

Ph- (CH<sub>2</sub>)<sub>4</sub>-Mg-Br

RN 207226-37-7 HCAPLUS

CN Benzene, 2-ethenyl-1,3-difluoro- (9CI) (CA INDEX NAME)

RN 274918-51-3 HCAPLUS

CN L-Proline, N-[(1,1-dimethylethoxy)carbonyl]-L- $\alpha$ -aspartyl-L- $\alpha$ glutamyl-L-valyl-L-valyl-, 1,2-bis(1,1-dimethylethyl) ester (9CI) INDEX NAME)

THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: 25 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2001:78359 HCAPLUS

DOCUMENT NUMBER:

134:147855

TITLE:

Preparation of lactam acylaminoalkaneboronates as

inhibitors of hepatitis C virus NS3 protease.

INVENTOR(S):

Priestley, E. Scott; Decicco, Carl

PATENT ASSIGNEE(S):

Du Pont Pharmaceuticals Company, USA

PCT Int. Appl., 130 pp. SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE:

LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

· ]	PATENT NO.					ND	DATE			APPLICATION NO.					DATE				
1	WO 2001007407				A1		20010201			WO 2000-US201				 89	9 20000726				
	W	<i>:</i>	AU,	BR,	CA,	CN,	CZ,	EE,	HU,	IL,	IN,	JP,	KR,	LT,	LV,	MX,	NO,	NZ,	
			PL,	RO,	SG,	SI,	SK,	TR,	UA,	VN,	ZA,	AM,	AZ,	BY,	KG,	KΖ,	MD,	RU,	
			ТJ,	TM															
	R	: W	AT,	BE,	CH,	CY,	DE,	DK,	ES,	FΙ,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	
			PT,	SE															
I	EP 1206449				A1 20020522					EP 2000-950642					20000726				
	R	:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙΤ,	LI,	LU,	NL,	SE,	MC,	PT,	
			IE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL								
PRIORITY APPLN. INFO.:					Ţ				JS 1999-145631P P				P	19990726					
						V				NO 2000-US20189			W	20000726					
OTHER SOURCE(S): GI							MARPAT 134:147855												

AB Title compds. [I; X = B(OH)2, BYY1, COCONHR1a; Y1, Y2 = OH, F, amino, alkoxy; BY1Y2 = atoms to form a cyclic boron ester, amide, or amide-ester containing 2-20 C atoms and optionally 1-3 N, O, or S atoms; R1, R1a = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl; R2 = H; R1R2C = cycloalkyl; R3 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, Ph, naphthyl, heteroaryl; R4 = H, (substituted) alkyl, Ph, PhCH2, PhCH2CH2; R5 = H, QR5a; Q = chain of 0-3 amino acids; R5a = SOR6, SO2R7, COR6, CO2R8; R6 = (substituted) alkyl, Ph, naphthyl, PhCH2, heteroaryl; R7 = H, alkyl; R8 = alkyl, PhCH2, cycloalkylmethyl; Q = (CH2)1-3], were prepared Thus, (1R)-1-[[(2S)-3-cyclohexyl-2-[3-isopropyl-3-[[(2S)-3-methyl-2-[(2-pyrazinylcarbonyl)amino]butanoyl]amino]-2-oxo-1-pyrrolidinyl]propanoyl]amino]-3-butenylboronic acid (+)-pinanediol ester was prepared by solution phase chemical A number of I inhibited hepatitis C virus

NS3 protease with Ki<60  $\mu M$ .

IT 149885-80-3

RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)

(inhibitors; preparation of lactam acylaminoalkaneboronates as inhibitors of hepatitis C virus NS3 protease)

RN 149885-80-3 HCAPLUS

CN Proteinase, polyprotein-processing, NS3 (9CI) (CA INDEX NAME)

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*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
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IT 323196-84-5P 323196-85-6P 323196-86-7P 323196-87-8P 323196-88-9P 323196-89-0P 323196-90-3P 323196-91-4P 323196-92-5P 323196-93-6P 323196-94-7P 323196-95-8P 323196-96-9P 323196-97-0P 323196-98-1P 323196-99-2P 323197-00-8P 323197-01-9P

323197-02-0P 323197-03-1P 323197-04-2P

323197-05-3P 323197-06-4P 323197-07-5P

323197-08-6P 323197-09-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

RN 323196-84-5 HCAPLUS

CN Pyrazinecarboxamide, N-[(1S)-1-[[[1-[(1S)-1-(cyclohexylmethyl)-2-[[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]-3-butenyl]amino]-2-oxoethyl]-3-(1-methylethyl)-2-oxo-3-pyrrolidinyl]amino]carbonyl]-2-methylpropyl]- (9CI) (CA INDEX NAME)

RN 323196-85-6 HCAPLUS

CN Pyrazinecarboxamide, N-[(1S)-1-[[[1-[(1S)-1-(cyclohexylmethyl)-2-[[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]-3-butenyl]amino]-2-oxoethyl]-3-(1-methylethyl)-2-oxo-3-piperidinyl]amino]carbonyl]-2-methylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323196-86-7 HCAPLUS

CN 1H-Azepine-1-acetamide, N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]hexahydro-3-[(methylsulfonyl)amino]-2-oxo-(9CI) (CA INDEX NAME)

RN 323196-87-8 HCAPLUS

CN 1-Pyrrolidineacetamide, 3-amino- $\alpha$ -(cyclohexylmethyl)-N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-2-oxo-, monohydrochloride, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 323196-88-9 HCAPLUS

CN 1-Pyrrolidineacetamide,  $3-[([1,1'-biphenyl]-4-ylsulfonyl)amino]-\alpha-(cyclohexylmethyl)-N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-2-oxo-, (<math>\alpha$ S)- (9CI) (CA INDEX NAME)

RN 323196-89-0 HCAPLUS

CN 1-Pyrrolidineacetamide,  $\alpha$ -(cyclohexylmethyl)-N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-2-oxo-3-[[(4-propylphenyl)sulfonyl]amino]-,  $(\alpha S)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323196-90-3 HCAPLUS

CN 1-Pyrrolidineacetamide,  $\alpha$ -(cyclohexylmethyl)-N-[(1R)-1-[(3aS, 4S, 6S, 7aR)-hexahydro-3a, 5, 5-trimethyl-4, 6-methano-1, 3, 2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-3-[(1-naphthalenylsulfonyl)amino]-2-oxo-,  $(\alpha S)$ - (9CI) (CA INDEX NAME)

RN 323196-91-4 HCAPLUS

CN 1-Pyrrolidineacetamide,  $\alpha$ -(cyclohexylmethyl)-N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-2-oxo-3-[[(phenylamino)carbonyl]amino]-,  $(\alpha S)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323196-92-5 HCAPLUS

CN 1-Pyrrolidineacetamide, α-(cyclohexylmethyl)-N-[(1R)-1[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-3-[[(3-methylphenyl)sulfonyl]amino]-2-oxo-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323196-93-6 HCAPLUS

CN Boronic acid, [(1R)-1-[[(2S)-3-cyclohexyl-2-[3-(1-methylethyl)-3-[[(3-methylphenyl)sulfonyl]amino]-2-oxo-1-pyrrolidinyl]-1-oxopropyl]amino]propyl]- (9CI) (CA INDEX NAME)

RN 323196-94-7 HCAPLUS

CN Carbamic acid, [1-[(1S)-2-[[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]amino]-2-oxo-1-phenylethyl]-3-(1-methylethyl)-2-oxo-3-pyrrolidinyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323196-95-8 HCAPLUS

CN 1-Pyrrolidineacetamide, 3-amino-N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-2-oxo-α-phenyl-, monohydrochloride, (αS)- (9CI) (CA INDEX NAME)

RN 323196-96-9 HCAPLUS

CN 1-Pyrrolidineacetamide, N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-3-[(methylsulfonyl)amino]-2-oxo- $\alpha$ -phenyl-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323196-97-0 HCAPLUS

CN 1-Pyrrolidineacetamide, N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-2-oxo-α-phenyl-3-[[(4-propylphenyl)sulfonyl]amino]-, (αS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323196-98-1 HCAPLUS

CN Carbamic acid, [1-[(1S)-1-[[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-

trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]amino]carbonyl]-3methylbutyl]-3-(1-methylethyl)-2-oxo-3-pyrrolidinyl]-, phenylmethyl ester
(9CI) (CA INDEX NAME)

## Absolute stereochemistry.

RN 323196-99-2 HCAPLUS

CN 1-Pyrrolidineacetamide, 3-amino-N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-α-(2-methylpropyl)-2-oxo-, monohydrochloride, (αS)- (9CI) (CA INDEX NAME)

# Absolute stereochemistry.

# ● HCl

RN 323197-00-8 HCAPLUS

CN 1-Pyrrolidineacetamide, N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-\alpha-(2-methylpropyl)-3-[(methylsulfonyl)amino]-2-oxo-, (\alphaS)-(9CI) (CA INDEX NAME)

RN 323197-01-9 HCAPLUS

CN 1-Pyrrolidineacetamide, N-[(1R)-1-[(3aS, 4S, 6S, 7aR)-hexahydro-3a, 5, 5-trimethyl-4, 6-methano-1, 3, 2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)- $\alpha$ -(2-methylpropyl)-2-oxo-3-[[(4-propylphenyl)sulfonyl]amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-02-0 HCAPLUS

CN Pyrazinecarboxamide, N-[(1S)-1-[[[1-[(1S)-1-(cyclohexylmethyl)-2-[[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]-3-butenyl]amino]-2-oxoethyl]-3-ethyl-2-oxo-3-pyrrolidinyl]amino]carbonyl]-2-methylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-03-1 HCAPLUS

CN Carbamic acid, [1-[(1S)-1-(cyclohexylmethyl)-2-[[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]amino]-2-oxoethyl]-3-(1-methylethyl)-2-oxo-3-piperidinyl]-,

phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-04-2 HCAPLUS

CN Carbamic acid, [1-[(1S)-2-[[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]amino]-2-oxo-1-phenylethyl]-3-(1-methylethyl)-2-oxo-3-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-05-3 HCAPLUS

CN 1-Piperidineacetamide, 3-amino-N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-2-oxo- $\alpha$ -phenyl-, monohydrochloride, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 323197-06-4 HCAPLUS

CN Carbamic acid, [1-[(1S)-2-[[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]amino]-2-oxo-1-phenylethyl]-3-(1-methylethyl)-2-oxo-3-piperidinyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-07-5 HCAPLUS

CN 1-Piperidineacetamide, 3-(benzoylamino)-N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-2-oxo- $\alpha$ -phenyl-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-08-6 HCAPLUS

CN 1-Piperidineacetamide, N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-3-[(methylsulfonyl)amino]-2-oxo- $\alpha$ -phenyl-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

RN 323197-09-7 HCAPLUS

CN 1-Piperidineacetamide, N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-3-(1-methylethyl)-3-[[(3-methylphenyl)sulfonyl]amino]-2-oxo- $\alpha$ -phenyl-, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 85-46-1, 1-Naphthylsulfonyl chloride 98-88-4, Benzoyl chloride 103-71-9, Phenyl isocyanate, reactions 106-95-6 , Allyl bromide, reactions 108-98-5, Thiophenol, reactions 124-63-0, Methanesulfonyl chloride 359-07-9 460-37-7, 3,3,3-Trifluoropropyl iodide 931-59-9, Phenylsulfenyl chloride 1149-26-4 1623-93-4, 4-Biphenylsulfonyl chloride 1730-25-2, Allylmagnesium bromide **1899-93-0 3182-79-4 4333-56-6,** Cyclopropyl bromide 6009-07-0 13734-41-3 15028-39-4, L-Phenylglycine methyl ester hydrochloride 17193-39-4 18680-27-8 38329-34-9, L-Phenylglycine hydrochloride 42918-86-5 76347-13-2 84110-32-7 90084-27-8 119479-32-2 130653-09-7 146949-07-7 323197-58-6 323197-73-5 RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of lactam acylaminoalkaneboronates as inhibitors of hepatitis C virus NS3 protease) 85-46-1 HCAPLUS RN CN 1-Naphthalenesulfonyl chloride (7CI, 8CI, 9CI) (CA INDEX NAME)

RN 98-88-4 HCAPLUS CN Benzoyl chloride (8CI, 9CI) (CA INDEX NAME)

RN 103-71-9 HCAPLUS

CN Benzene, isocyanato- (9CI) (CA INDEX NAME)

RN 106-95-6 HCAPLUS

CN 1-Propene, 3-bromo- (9CI) (CA INDEX NAME)

 $Br-CH_2-CH-CH_2$ 

RN 108-98-5 HCAPLUS

CN Benzenethiol (8CI, 9CI) (CA INDEX NAME)



RN 124-63-0 HCAPLUS

CN Methanesulfonyl chloride (6CI, 8CI, 9CI) (CA INDEX NAME)

RN 359-07-9 HCAPLUS

CN Ethane, 2-bromo-1,1-difluoro- (7CI, 8CI, 9CI) (CA INDEX NAME)

RN 460-37-7 HCAPLUS

CN Propane, 1,1,1-trifluoro-3-iodo- (7CI, 8CI, 9CI) (CA INDEX NAME)

F3C-CH2-CH2I

RN 931-59-9 HCAPLUS

CN Benzenesulfenyl chloride (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Ph-S-Cl

RN 1149-26-4 HCAPLUS

CN L-Valine, N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 1623-93-4 HCAPLUS

CN [1,1'-Biphenyl]-4-sulfonyl chloride (9CI) (CA INDEX NAME)

RN 1730-25-2 HCAPLUS

CN Magnesium, bromo-2-propenyl- (9CI) (CA INDEX NAME)

RN 1899-93-0 HCAPLUS

CN Benzenesulfonyl chloride, 3-methyl- (9CI) (CA INDEX NAME)

RN 3182-79-4 HCAPLUS

CN Glycine, N-2-propenyl-, ethyl ester (9CI) (CA INDEX NAME)

$$\overset{\text{O}}{\underset{\text{EtO}-\text{C-CH}_2-\text{NH-CH}_2-\text{CH}^-}{\text{CH}_2}} \text{CH}_2$$

RN 4333-56-6 HCAPLUS

CN Cyclopropane, bromo- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Br

RN 6009-07-0 HCAPLUS

CN Disulfide, chloro phenyl (8CI, 9CI) (CA INDEX NAME)

Phs-s-Cl

RN 13734-41-3 HCAPLUS

CN L-Valine, N-[(1,1-dimethylethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 15028-39-4 HCAPLUS

CN Benzeneacetic acid,  $\alpha$ -amino-, methyl ester, hydrochloride,  $(\alpha S)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

● HCl

RN 17193-39-4 HCAPLUS

CN Cyclohexanepropanoic acid,  $\alpha$ -amino-, methyl ester, hydrochloride,  $(\alpha S)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 18680-27-8 HCAPLUS CN Bicyclo[3.1.1]heptane-2,3-diol, 2,6,6-trimethyl-, (1S,2S,3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 38329-34-9 HCAPLUS CN Benzeneacetic acid,  $\alpha$ -amino-, hydrochloride,  $(\alpha S)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

● HCl

RN 42918-86-5 HCAPLUS CN Butanoic acid, 2-[[(phenylmethoxy)carbonyl]amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 76347-13-2 HCAPLUS

CN 1,3,2-Dioxaborolane, 4,4,5,5-tetramethyl-2-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 84110-32-7 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole, 2-ethenylhexahydro-3a,5,5-trimethyl-, (3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 90084-27-8 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole, 2-[(1S)-1-chloro-2-(phenylmethoxy)ethyl]hexahydro-3a,5,5-trimethyl-, (3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 119479-32-2 HCAPLUS

CN 4-Pentenoic acid, 2-[[(1,1-dimethylethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)

RN 130653-09-7 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole, 2-(1-chloroethenyl)hexahydro-3a,5,5-trimethyl-, (3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

RN 146949-07-7 HCAPLUS

CN Benzenesulfonyl chloride, 4-propyl- (9CI) (CA INDEX NAME)

RN 323197-58-6 HCAPLUS

CN L-Valine, N-(pyrazinylcarbonyl) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-73-5 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole-2-methanamine, hexahydro-3a,5,5-trimethyl- $\alpha$ -2-propenyl-, ( $\alpha$ R,3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

```
ΙT
     66080-23-7P 66866-64-6P 70557-99-2P
     83622-42-8P 94242-86-1P 95656-94-3P
     126689-01-8P 131357-48-7P 131433-93-7P
     172096-96-7P 319009-74-0P 319009-76-2P
     319009-78-4P 319009-80-8P 319009-82-0P
     319009-90-0P 319009-92-2P 319009-94-4P
     319009-96-6P 319009-98-8P 319010-99-6P
     319011-02-4P 319011-08-0P 319011-10-4P
     319011-16-0P 319011-18-2P 319011-22-8P
     319011-25-1P 319011-27-3P 319011-29-5P
     323197-10-0P 323197-11-1P 323197-12-2P
     323197-13-3P 323197-14-4P 323197-15-5P
     323197-16-6P 323197-17-7P 323197-18-8P
     323197-19-9P 323197-20-2P 323197-21-3P
     323197-22-4P 323197-23-5P 323197-24-6P
     323197-25-7P 323197-26-8P 323197-27-9P
     323197-28-0P 323197-29-1P 323197-30-4P
     323197-31-5P 323197-32-6P 323197-33-7P
     323197-34-8P 323197-35-9P 323197-36-0P
     323197-37-1P 323197-38-2P 323197-39-3P
     323197-40-6P 323197-41-7P 323197-42-8P
     323197-43-9P 323197-44-0P 323197-45-1P
     323197-46-2P 323197-47-3P 323197-48-4P
     323197-74-6P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of lactam acylaminoalkaneboronates as inhibitors of hepatitis C
        virus NS3 protease)
RN
     66080-23-7 HCAPLUS
CN
     1,3,2-Dioxaborolane, 4,4,5,5-tetramethyl-2-[(phenylthio)methyl]- (9CI)
     (CA INDEX NAME)
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RN 66866-64-6 HCAPLUS
CN 3-Oxazolidinecarboxylic acid, 4-(1-methylethyl)-5-oxo-, phenylmethyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 70557-99-2 HCAPLUS CN 1,3,2-Dioxaborolane, 2-(iodomethyl)-4,4,5,5-tetramethyl- (9CI) (CA INDEX

NAME)

RN 83622-42-8 HCAPLUS

CN 1,3,2-Dioxaborolane, 2-(chloromethyl)-4,4,5,5-tetramethyl- (9CI) (CA INDEX NAME)

RN 94242-86-1 HCAPLUS

CN 1,3,2-Dioxaborolane, 2-(1-chloroethyl)-4,4,5,5-tetramethyl- (9CI) (CA INDEX NAME)

RN 95656-94-3 HCAPLUS

CN 3-Oxazolidinecarboxylic acid, 4-ethyl-5-oxo-, phenylmethyl ester, (4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 126689-01-8 HCAPLUS

CN 1,3,2-Dioxaborolane, 2-cyclopropyl-4,4,5,5-tetramethyl- (9CI) (CA INDEX NAME)

RN 131357-48-7 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole, 2-[(1S)-1-chloro-3-butenyl]hexahydro-3a,5,5-trimethyl-, (3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 131433-93-7 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole, hexahydro-3a,5,5-trimethyl-2-(2-propenyl)-, (3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 172096-96-7 HCAPLUS

CN 3-Oxazolidinecarboxylic acid, 4-(1-methylethyl)-5-oxo-, 1,1-dimethylethyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 319009-74-0 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole-2-methanamine, hexahydro-3a,5,5-

trimethyl- $\alpha$ -[1-(phenylmethoxy)ethyl]-, hydrochloride, ( $\alpha$ R, 3aS, 4S, 6S, 7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 319009-76-2 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole-2-methanamine, hexahydro-3a,5,5-trimethyl- $\alpha$ -[(phenylmethoxy)methyl]-, hydrochloride, ( $\alpha$ R,3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 319009-78-4 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole-2-methanamine, hexahydro-3a,5,5-trimethyl- $\alpha$ -[(phenylthio)methyl]-, hydrochloride, (3aS,4S,6S,7aR)-(9CI) (CA INDEX NAME)

RN 319009-80-8 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole-2-methanamine, hexahydro-3a,5,5-trimethyl- $\alpha$ -[(phenyldithio)methyl]-, (3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 319009-82-0 HCAPLUS

CN 1,3,2-Dioxaborolane-2-methanamine, 4,4,5,5-tetramethyl- $\alpha$ -(3,3,3-trifluoropropyl)- (9CI) (CA INDEX NAME)

RN 319009-90-0 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole-2-methanamine, hexahydro-3a,5,5-trimethyl- $\alpha$ -2-propenyl-, hydrochloride, ( $\alpha$ R,3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

RN 319009-92-2 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole-2-methanamine,  $\alpha$ -ethylhexahydro-3a,5,5-trimethyl-, hydrochloride,  $(\alpha R, 3aS, 4S, 6S, 7aR)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

## ● HCl

RN 319009-94-4 HCAPLUS

CN 1,3,2-Dioxaborolane-2-methanamine,  $\alpha$ -cyclopropyl-4,4,5,5-tetramethyl-(9CI) (CA INDEX NAME)

RN 319009-96-6 HCAPLUS

CN 1,3,2-Dioxaborolane-2-methanamine,  $\alpha$ -(2,2-difluoroethyl)-4,4,5,5-tetramethyl-, hydrochloride (9CI) (CA INDEX NAME)

RN 319009-98-8 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole-2-methanamine,  $\alpha$ -ethenylhexahydro-3a,5,5-trimethyl-, hydrochloride, ( $\alpha$ R,3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

## ● HCl

RN 319010-99-6 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole, 2-[(1S)-1-chloropropyl]hexahydro-3a,5,5-trimethyl-, (3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 319011-02-4 HCAPLUS

CN 1,3,2-Dioxaborolane, 2-(chlorocyclopropylmethyl)-4,4,5,5-tetramethyl-(9CI) (CA INDEX NAME)

RN 319011-08-0 HCAPLUS

CN 1,3,2-Dioxaborolane, 2-[3,3-difluoro-1-(phenylthio)propyl]-4,4,5,5-tetramethyl- (9CI) (CA INDEX NAME)

RN 319011-10-4 HCAPLUS

CN 1,3,2-Dioxaborolane, 2-(3,3-difluoro-1-iodopropyl)-4,4,5,5-tetramethyl-(9CI) (CA INDEX NAME)

RN 319011-16-0 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole, hexahydro-3a,5,5-trimethyl-2-[1-(phenylmethoxy)ethyl]-, (3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 319011-18-2 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole, 2-[(1S)-1-chloro-2-(phenylmethoxy)propyl]hexahydro-3a,5,5-trimethyl-, (3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 319011-22-8 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole, 2-[1-chloro-2-(phenylthio)ethyl]hexahydro-3a,5,5-trimethyl-, (3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 319011-25-1 HCAPLUS

CN

4,6-Methano-1,3,2-benzodioxaborole, 2-[1-chloro-2-(phenyldithio)ethyl]hexahydro-3a,5,5-trimethyl-, (3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 319011-27-3 HCAPLUS

CN 1,3,2-Dioxaborolane, 4,4,5,5-tetramethyl-2-[4,4,4-trifluoro-1-(phenylthio)butyl]- (9CI) (CA INDEX NAME)

RN 319011-29-5 HCAPLUS
CN 1.3.2-Dioxaborolane, 4.4.5.5-tetramethy

CN 1,3,2-Dioxaborolane, 4,4,5,5-tetramethyl-2-(4,4,4-trifluoro-1-iodobutyl)-(9CI) (CA INDEX NAME)

RN 323197-10-0 HCAPLUS

CN 3-Oxazolidinecarboxylic acid, 4-(1-methylethyl)-5-oxo-4-(2-propenyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|cccc} O & & & & & \\ C-O-CH_2 & Ph & & & & \\ & & & Pr-i & & \\ O & & & CH_2-CH-CH_2 \\ & & & & O \end{array}$$

RN 323197-11-1 HCAPLUS

CN 4-Pentenoic acid, 2-(1-methylethyl)-2-[[(phenylmethoxy)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 323197-12-2 HCAPLUS

CN Valine, 2-(2-oxoethyl)-N-[(phenylmethoxy)carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 323197-13-3 HCAPLUS

CN 1-Pyrrolidineacetic acid,  $\alpha$ -(cyclohexylmethyl)-3-(1-methylethyl)-2-oxo-3-[[(phenylmethoxy)carbonyl]amino]-, methyl ester, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-14-4 HCAPLUS

CN 1-Pyrrolidineacetic acid, 3-amino- $\alpha$ -(cyclohexylmethyl)-3-(1-methylethyl)-2-oxo-, methyl ester, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-15-5 HCAPLUS

CN 1-Pyrrolidineacetic acid,  $\alpha$ -(cyclohexylmethyl)-3-(1-methylethyl)-3-[(2S)-3-methyl-1-oxo-2-[(pyrazinylcarbonyl)amino]butyl]amino]-2-oxo-, methyl ester,  $(\alpha S)$ - (9CI) (CA INDEX NAME)

RN 323197-16-6 HCAPLUS

CN 1-Pyrrolidineacetic acid,  $\alpha$ -(cyclohexylmethyl)-3-(1-methylethyl)-3-[(2S)-3-methyl-1-oxo-2-[(pyrazinylcarbonyl)amino]butyl]amino]-2-oxo-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-17-7 HCAPLUS

CN Norvaline, 5-hydroxy-2-(1-methylethyl)-N-[(phenylmethoxy)carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 323197-18-8 HCAPLUS

CN Norvaline, 2-(1-methylethyl)-5-oxo-N-[(phenylmethoxy)carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 323197-19-9 HCAPLUS

CN Cyclohexanepropanoic acid,  $\alpha$ -[[4-(methoxycarbonyl)-5-methyl-4-[[(phenylmethoxy)carbonyl]amino]hexyl]amino]-, methyl ester, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-20-2 HCAPLUS

CN 1-Piperidineacetic acid,  $\alpha$ -(cyclohexylmethyl)-3-(1-methylethyl)-2-oxo-3-[[(phenylmethoxy)carbonyl]amino]-, methyl ester, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-21-3 HCAPLUS

CN 1-Piperidineacetic acid, 3-amino- $\alpha$ -(cyclohexylmethyl)-3-(1-methylethyl)-2-oxo-, methyl ester, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

RN 323197-22-4 HCAPLUS

CN l-Piperidineacetic acid,  $\alpha$ -(cyclohexylmethyl)-3-(1-methylethyl)-3-[(2S)-3-methyl-1-oxo-2-[(pyrazinylcarbonyl)amino]butyl]amino]-2-oxo-, methyl ester, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-23-5 HCAPLUS

CN 1-Piperidineacetic acid,  $\alpha$ -(cyclohexylmethyl)-3-(1-methylethyl)-3-[(2S)-3-methyl-1-oxo-2-[(pyrazinylcarbonyl)amino]butyl]amino]-2-oxo-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-24-6 HCAPLUS

CN Glycine, 4,5-didehydro-N-[(1,1-dimethylethoxy)carbonyl]norvalyl-N-2-propenyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 323197-25-7 HCAPLUS

CN 1H-Azepine-1-acetic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2,3,4,7-tetrahydro-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)

RN 323197-26-8 HCAPLUS

CN 1H-Azepine-1-acetic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-2,3,4,7-tetrahydro-2-oxo- (9CI) (CA INDEX NAME)

RN 323197-27-9 HCAPLUS

CN Carbamic acid, [1-[2-[[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]amino]-2-oxoethyl]hexahydro-2-oxo-1H-azepin-3-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-28-0 HCAPLUS

CN 1H-Azepine-1-acetamide, 3-amino-N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]hexahydro-2-

oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-29-1 HCAPLUS

CN 1-Pyrrolidineacetic acid,  $\alpha$ -(cyclohexylmethyl)-3-(1-methylethyl)-2-oxo-3-[[(phenylmethoxy)carbonyl]amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-30-4 HCAPLUS

CN Carbamic acid, [1-[(1S)-1-(cyclohexylmethyl)-2-[[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]amino]-2-oxoethyl]-3-(1-methylethyl)-2-oxo-3-pyrrolidinyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 323197-31-5 HCAPLUS

CN 1-Pyrrolidineacetic acid, 3-(1-methylethyl)-2-oxo- $\alpha$ -phenyl-3-[[(phenylmethoxy)carbonyl]amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-32-6 HCAPLUS

CN 1-Pyrrolidineacetic acid, 3-(1-methylethyl)- $\alpha$ -(2-methylpropyl)-2-oxo-3-[[(phenylmethoxy)carbonyl]amino]-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-33-7 HCAPLUS

CN 3-Oxazolidinecarboxylic acid, 4-ethyl-5-oxo-4-(2-propenyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
O \\
C-O-CH_2-Ph \\
\downarrow \\
Et \\
O \\
O \\
CH_2-CH=-CH_2
\end{array}$$

$$\begin{array}{c} \text{O} \\ || \\ \text{C-OMe} \\ || \\ \text{Et-C-CH}_2\text{-CH----} \text{CH}_2 \\ || \\ \text{NH-C-O-CH}_2 \quad \text{Ph} \\ || \\ \text{O} \end{array}$$

RN 323197-35-9 HCAPLUS
CN Butanoic acid, 2-ethyl-4-oxo-2-[[(phenylmethoxy)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{O} \\ || \\ \text{C--OMe} \\ || \\ \text{Et--C--CH}_2\text{---CHO} \\ || \\ \text{NH--C--O--CH}_2\text{---Ph} \\ || \\ \text{O} \end{array}$$

RN 323197-36-0 HCAPLUS CN 1-Pyrrolidineacetic acid,  $\alpha$ -(cyclohexylmethyl)-3-ethyl-2-oxo-3-[[(phenylmethoxy)carbonyl]amino]-, methyl ester, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

RN 323197-37-1 HCAPLUS CN 1-Pyrrolidineacetic acid, 3-amino- $\alpha$ -(cyclohexylmethyl)-3-ethyl-2-oxo-, methyl ester, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-38-2 HCAPLUS

CN 1-Pyrrolidineacetic acid,  $\alpha$ -(cyclohexylmethyl)-3-ethyl-3-[[(2S)-3-methyl-1-oxo-2-[(pyrazinylcarbonyl)amino]butyl]amino]-2-oxo-, methyl ester, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

RN 323197-39-3 HCAPLUS

CN 1-Pyrrolidineacetic acid,  $\alpha$ -(cyclohexylmethyl)-3-ethyl-3-[[(2S)-3-methyl-1-oxo-2-[(pyrazinylcarbonyl)amino]butyl]amino]-2-oxo-, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-40-6 HCAPLUS

CN 3-Oxazolidinecarboxylic acid, 4-(1-methylethyl)-5-oxo-4-(2-propenyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 323197-41-7 HCAPLUS

CN 4-Pentenoic acid, 2-[[(1,1-dimethylethoxy)carbonyl]amino]-2-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 323197-42-8 HCAPLUS

CN 4-Pentenoic acid, 2-[[(1,1-dimethylethoxy)carbonyl]amino]-2-(1-methylethyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 323197-43-9 HCAPLUS

CN Norvaline, N-[(1,1-dimethylethoxy)carbonyl]-5-hydroxy-2-(1-methylethyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 323197-44-0 HCAPLUS

CN Norvaline, N-[(1,1-dimethylethoxy)carbonyl]-2-(1-methylethyl)-5-oxo-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 323197-45-1 HCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[[4-[[(1,1-dimethylethoxy)carbonyl]amino]-5-methyl-4-[(phenylmethoxy)carbonyl]hexyl]amino]-, methyl ester, ( $\alpha$ S)-(9CI) (CA INDEX NAME)

RN 323197-46-2 HCAPLUS

CN Benzeneacetic acid,  $\alpha$ -[[4-carboxy-4-[[(1,1-dimethylethoxy)carbonyl]amino]-5-methylhexyl]amino]-, monomethyl ester, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-47-3 HCAPLUS

CN 1-Piperidineacetic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-methylethyl)-2-oxo- $\alpha$ -phenyl-, methyl ester, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-48-4 HCAPLUS

CN 1-Piperidineacetic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(1-methylethyl)-2-oxo- $\alpha$ -phenyl-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 323197-74-6 HCAPLUS

CN 1-Pyrrolidineacetic acid, 3-(1-methylethyl)-2-oxo-α-phenyl-3[[(phenylmethoxy)carbonyl]amino]-, methyl ester, (αS)- (9CI) (CA
INDEX NAME)

REFERENCE COUNT:

12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2000:607748 HCAPLUS

DOCUMENT NUMBER:

133:335259

TITLE:

1-Aminocyclopropaneboronic Acid: Synthesis and

Incorporation into an Inhibitor of Hepatitis C Virus

NS3 Protease

AUTHOR(S):

Priestley, E. Scott; Decicco, Carl

CORPORATE SOURCE:

Department of Chemical and Physical Sciences, DuPont Pharmaceuticals Company, Wilmington, DE, 19880, USA

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Organic Letters (2000), 2(20), 3095-3097 CODEN: ORLEF7; ISSN: 1523-7060

American Chemical Society

PUBLISHER:

Journal

DOCUMENT TYPE:

English

LANGUAGE:

OTHER SOURCE(S):

CASREACT 133:335259

The previously unreported  $\alpha, \alpha$ -disubstituted 1-aminoboronate esters have potential utility in peptidomimetic design, particularly against serine protease targets. A concise synthesis of 1-aminocyclopropaneboronate pinanediol ester is reported, and a peptidyl derivative has modest affinity ( $Ki = 1.6 \mu M$ ) for hepatitis C NS3 protease. Analogs with iso-Pr and cyclohexyl in place of cyclopropyl were also prepared and tested.

274918-51-3, Boc-Asp(O-t-Bu)-Glu(O-t-Bu)-Val-Val-Pro-OH ΙT RL: RCT (Reactant); RACT (Reactant or reagent)

(coupling with  $\alpha, \alpha$ -disubstituted 1-aminoboronate esters)

274918-51-3 HCAPLUS RN

L-Proline, N-[(1,1-dimethylethoxy)carbonyl]-L- $\alpha$ -aspartyl-L- $\alpha$ -CN glutamyl-L-valyl-, 1,2-bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Cyclopropane, isocyano- (9CI) (CA INDEX NAME)

NH-CHO

58644-53-4P, Cyclopropyl isocyanide RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (explosion hazard during reaction; preparation and lithiation followed by metathesis with triisopropyl borate in preparation of  $\alpha, \alpha$ -disubstituted 1-aminoboronate ester)

RN 58644-53-4 HCAPLUS

CN

IT 5419-55-6, Triisopropyl borate 18680-27-8 RL: RCT (Reactant); RACT (Reactant or reagent) (for preparation of  $\alpha, \alpha$ -disubstituted 1-aminoboronate esters) RN 5419-55-6 HCAPLUS (Boric acid (H3BO3), tris(1-methylethyl) ester (9CI) (CA INDEX NAME)

18680-27-8 HCAPLUS RN

Bicyclo[3.1.1]heptane-2,3-diol, 2,6,6-trimethyl-, (1S,2S,3R,5S)- (9CI) CN (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

ΙT 149885-80-3, NS3 Protease

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(hepatitis C virus; synthesis of  $\alpha, \alpha$ -disubstituted

1-aminoboronate esters and incorporation into inhibitor of)

RN 149885-80-3 HCAPLUS

Proteinase, polyprotein-processing, NS3 (9CI) (CA INDEX NAME) CN

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

598-45-8, Isopropyl isocyanide 931-53-3, Cyclohexyl

isocyanide

RL: RCT (Reactant); RACT (Reactant or reagent)

(lithiation followed by metathesis with triisopropyl borate in preparation

of  $\alpha$ ,  $\alpha$ -disubstituted 1-aminoboronate ester)

RN 598-45-8 HCAPLUS

Propane, 2-isocyano- (9CI) (CA INDEX NAME) CN

931-53-3 HCAPLUS RN

Cyclohexane, isocyano- (9CI) (CA INDEX NAME) CN

303191-80-2P 303191-81-3P 303191-82-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and activity as inhibitor of hepatitis C NS3 protease)

RN 303191-80-2 HCAPLUS

L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N-[1-[(3aS, 4S, 6S, 7aR) -hexahydro-3a, 5, 5-trimethyl-4, 6-methano-1, 3, 2-benzodioxaborol-2-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 303191-81-3 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N-[1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]-1-methylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 303191-82-4 HCAPLUS

CN L-Prolinamide, L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N-[1- [(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]cyclohexyl]- (9CI) (CA INDEX NAME)

IT 303191-71-1P 303191-72-2P 303191-73-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and conversion to amine hydrochloride using methanolic hydrogen chloride)

RN 303191-71-1 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole, hexahydro-2-(1-isocyanocyclopropyl)-3a,5,5-trimethyl-, (3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$-C = N + R$$

RN 303191-72-2 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole, hexahydro-2-(1-isocyano-1-methylethyl)-3a,5,5-trimethyl-, (3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

RN 303191-73-3 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborole, hexahydro-2-(1-isocyanocyclohexyl)-3a,5,5-trimethyl-, (3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 303191-74-4P 303191-75-5P 303191-76-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and coupling with pentapeptide)

RN 303191-74-4 HCAPLUS

CN Cyclopropanamine, 1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 303191-75-5 HCAPLUS

CN 4,6-Methano-1,3,2-benzodioxaborol-2-methanamine, hexahydro- $\alpha$ , $\alpha$ ,3a,5,5-pentamethyl-, hydrochloride, (3aS,4S,6S,7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 303191-76-6 HCAPLUS

CN Cyclohexanamine, 1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

IT 303191-77-7P 303191-78-8P 303191-79-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and deprotection of)

RN 303191-77-7 HCAPLUS

CN L-Prolinamide, N-[(1,1-dimethylethoxy)carbonyl]-L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N-[1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]cyclopropyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

RN 303191-78-8 HCAPLUS

CN L-Prolinamide, N-[(1,1-dimethylethoxy)carbonyl]-L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N-[1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]-1-methylethyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

RN 303191-79-9 HCAPLUS

CN L-Prolinamide, N-[(1,1-dimethylethoxy)carbonyl]-L- $\alpha$ -aspartyl-L- $\alpha$ -glutamyl-L-valyl-L-valyl-N-[1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]cyclohexyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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